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Study of DM interaction in triangular lattice

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Abstract : We have studied the triangular lattice using linear spin-wave theory with Heisenberg antiferromagnets in addition to Dzyaloshinskii-Moriya interaction and weak magnetic field. The quantum corrections to the ground state energy and sublattice magnetization has been calculated analytically as a function of DM interaction strength and also of the magnetic field. The gap in the excitation spectrum has also been calculated. Finally, we come to the conclusion that the DM interaction stabilizes the LRO reducing the effect of the quantum fluctuation.

Keywords : Triangular lattice, Dzyaloshinskii-Moriya interaction.

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1. Introduction

In the last few decades, geometrically frustrated antiferromagnets (AFM) have come to be very important for both experimental and theoretical research. The most extensively studied systems are the triangular and kagomé lattice AFM in two dimensions and pyrochlore lattice in three dimensions. A large number of studies have been devoted to the triangular lattice. P W Anderson [1] first proposed that the system has a spin-disordered ground state similar to the frustrated square lattices with further neighbor exchange, along with the usual nearest neighbor interaction. The resonating valence bond (RVB) state is one of the possible candidates for the ground state in this regime. An estimate of ground state energy has been obtained from various RVB-type variational wavefunctions [2,3] and also from the variational values of Huse and Elser. But several other methods, such as spin wave theory [4–6], variational calculation [7], exact diagonalization of small clusters [8] and Monte Carlo numerical method indicated the possibility of long range order with the ground state energy lower than the spin disordered states. The sublattice magnetization is, however, reduced considerably (~0.239) from its classical values (~0.5) due to the zero point quantum fluctuations. It is generally believed that the frustrated triangular lattice with Heisenberg antiferromagnet (HAFM) is quite similar to the square lattice *i.e.* a ground state with long range Néel ordered. Experimental realizations of triangular lattice HAFM are materials like VCl_2, VBr_2, $NaNiO_2$ *etc.* Possible ground state orderings in the quantum antiferromagnets

(QAFM) include Néel, helical, spin liquid, spin nematic, dimer or chiral liquid. The triangular QAFM is thought to exhibit long range 120° Néel order at $T = 0$. Dimer ordering is found for various SU(n) models for large n and may even survive in the $n \to 2$ limit, *i.e.* for $S = 1/2$, for models with competing further neighbor interactions Indeed there is no experimental realization or proof of LRO or spin liquid ground states The system like Cs_2CuCl_4 which is quasi-two dimensional $S = 1/2$ system on triangular lattice [9] shows a LRO at below the temperature 0.62 K and supposed to have the anisotropic Dzyaloshinskii-Moriya (DM) interaction. The DM interaction produces canting between the spins and a LRO in the form of an incommensurate spiral spin structure occurs below the Neel temperature at zero field.

There is a lot of controversy about the ground state of such frustrated lattices A large number of studies have been done in these lattices with Heisenberg Hamiltonian. In this work we have seen that anisotropic Heisenberg Hamiltonian stabilizes the LRO. In view of that, we have undertaken this study of Heisenberg model along with anisotropic DM interaction on triangular lattice It has been observed that the effect of quantum fluctuation in ground state energy and sublattice magnetization decreases as the strength of DM interaction increases In particular, we would like to study the effect of this anisotropic DM interaction on the ground state energy sublattice magnetization and gap in the excitation spectrum. Effect of external magnetic field has also been taken into account. This paper is organized as follows In Section II, we write the general Hamiltonian and the ground state of the lattice. In Section III we shall have the major steps of the calculation and the results. Then, in the last Section, we shall conclude with our results.

2. The Hamiltonian

The most general spin Hamiltonian for two neighboring spin-1/2 magnetic ions in case of the insulator is given by

$$H_{ij} = J_{ij} S_i \cdot S_j + D_{ij} \cdot S_i \times S_j + S_i \cdot A_{ij} \cdot S_j + hS_i . \tag{1}$$

The first term is the Heisenberg term. It is the symmetric part of the Hamiltonian. The second term is the anisotropic DM interaction and the in the last term $\boldsymbol{A}_{ij}$ is the anisotropic symmetric exchange interaction. The last term is the zeeman term. Here, the consequences of the DM interaction on the low temperature magnetic structure are explored in the case where $\boldsymbol{D}$ is perpendicular to the lattice plane. Taking into account the super exchange mechanism, the isotropic exchange J_{ij} is proportional to t_{ij}^2/U where t_{ij} is the inter site hopping and U is the onsite Coulomb repulsion. It was shown by Moriya that $|\boldsymbol{D}_{ij}|$ is proportional to $(\lambda t_{ij}^2/\Delta U)$ where λ is the spin orbit coupling and Δ is the crystal field splitting and $\boldsymbol{A}_{ij}$ is proportional to $(\lambda^2 t_{ij}^2/\Delta^2 U)$. The third term, for a small value of λ, being one order of magnitude smaller than DM interaction is neglected. The magnetic field is acting on the z-direction. Then finally we take the Hamiltonian as,

$$H = J\sum_{\langle i,j\rangle} S_i \cdot S_j + D\cdot \sum_{\langle i,j\rangle} S_i \times S_j + h\sum_i S_i . \tag{2}$$

We have taken this Hamiltonian on this lattice. At first the classical ground state has been investigated in the following.

In the classical limit ($S \to \infty$), the spins are treated as the classical vector oriented in the x-z plane. The DM interaction is along the y-direction. In a single triangular plaquette three spin vectors make angles 0, θ_1 and θ_2 with respect to some reference direction. Then the classical Hamiltonian in the ansence of the magnetic field, can be written as

$$E_{cl} = \frac{S^2}{\cos\phi}\left[\cos(\phi - \vartheta_1) + \cos(\phi - \vartheta_2) + \cos(\phi - \vartheta_2 + \vartheta_1)\right], \tag{3}$$

where $\varphi = \tan^{-1}(D/J)$. To obtain the classical ground state one has to minimize the above expression with respect to θ_1 and θ_2. Then two possible orientations are obtained as (i) $\theta_1 = 2\pi/3$, $\theta_2 = 4\pi/3$ for $\boldsymbol{D}$ is in negative y-direction and (ii) $\theta_1 = 4\pi/3$, $\theta_2 = 2\pi/3$ for $\boldsymbol{D}$ is in positive y-direction. Thus, we can conclude that the classical ground state is 120° Néel ordered and the direction of the DM interaction changes the chiralities of the ordering. In Figure 1 two possible ground states are shown. Now we study the effect of quantum fluctuation using the linear spin-wave theory in the presence of small magnetic field.

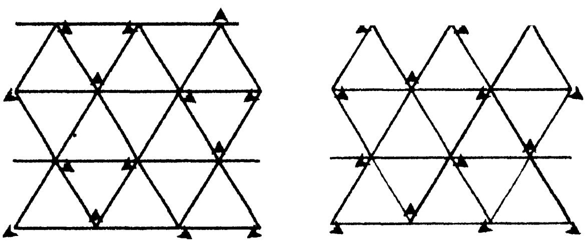

Figure 1. Two possible Néel orderings for positive and negative values of DM interaction acting perpendicular to the lattice plane in a triangular lattice.

3. Linear spin-wave theory

We consider the canted spin ordering, where spin vectors are oriented in the x-z plane. To bring the neighboring spins in the direction of same magnetization axis (say z-axis), one should rotate all the spins about y-axis and in the new reference frame the spin are defined as

$$S_i^{x'} = \cos Q S_i^x + \sin Q S_i^z,$$

$$S_i^{y'} = S_i^y.$$

$$S_i^{z'} = -\sin Q S_i^x + \cos Q S_i^z, \tag{4}$$

where Q is the angle of the spin vectors with respect to the z-direction. In this new description we take the Holstein Primakoff transformation, as

$$S_i^x = \frac{1}{2}\sqrt{2S}(a_i + a_i^+)\,; \quad S_i^y = \frac{1}{2}\sqrt{2S}(a_i - a_i^+)\,; \quad S_i^z = (S - a_i^+ a_i)\,. \tag{5}$$

To study the excitation spectrum, these bosons are again transformed to the Fourier space by

$$a_k = \frac{1}{\sqrt{N}} \sum_i e^{ik r_i} a_i\,, \tag{6}$$

where N is the number of lattice points belonging to one sublattice. Here, we consider the nearest neighbor interaction only. Let J and D be the strength Heisenberg interaction and DM interaction strength. Triangular lattice is described as 120° Néel ordering and three types spins $A(Q = 0)$, $B(Q = 120°)$ and $C(Q = 240°)$ are possible belonging to three different sublattices. So for D positive, $Q_{\alpha\beta}$ is taken as $2\pi/3$ and for D negative, $Q_{\alpha\beta}$ is $4\pi/3$ and in this way, another ground state for different chirality has been taken into account. Every spin belonging to one particular sublattice, interacts with the other through the bond directions $r_1 = (1,0)$, $r_2 = (-1/2, \sqrt{3}/2)$ and $r_3 = (-1/2, -\sqrt{3}/2)$. We define the bosons of the sublattices A, B and C as a, b and c then we have the Hamiltonian as

$$H_k = \frac{9}{2} S^2(-J_1 + \sqrt{3}D_1) + 3hS + \frac{3S}{2} \sum_{\alpha,\beta,k} [(\alpha_k^+ \beta_k) H_0(k) \begin{pmatrix} \alpha_k \\ \beta_k^+ \end{pmatrix} - 3C_1]\,, \tag{7}$$

where

$$H_0(k) = \begin{bmatrix} M_1 & M_2 \\ M_2 & M_1 \end{bmatrix}, \tag{8}$$

$$M_1 = \begin{bmatrix} C_1 & C_2 z & C_2 z^* \\ C_2 z^* & C_1 & C_2 z \\ C_2 z & C_2 z^* & C_1 \end{bmatrix},$$

$$M_2 = C_3 \begin{bmatrix} 0 & z & z^* \\ z^* & 0 & z \\ z & z^* & 0 \end{bmatrix}, \tag{9}$$

$$z = \frac{1}{12}\left(e^{-ik r_1} + e^{-ik r_2} + e^{-ik r_3}\right), \tag{10}$$

$$\begin{aligned} C_1 &= -J - \sqrt{3}D - \frac{h}{3S}, \\ C_2 &= J - \sqrt{3}D, \\ C_3 &= -3J - \sqrt{3}D, \end{aligned} \tag{11}$$

$$\alpha_k^+ = \begin{pmatrix} a_k \\ b_k \\ c_k \end{pmatrix}; \beta_k = \alpha_{-k}\,. \tag{12}$$

Here, the 6 × 6 matrix $H_0(k)$ can be diagonalized analytically by general Bogoliubov transformation. It is interesting to note that all the 3 × 3 blocks building the matrix $H_0(k)$ are the permutation matrices and thus can be diagonalised simultaneously in the basis

$$u_1 = (1 \quad 1 \quad 1); \quad u_2 = \left(1 \quad j \quad j^2\right); \quad u_3 = \left(1 \quad j^2 \quad j\right) \text{ and } j = e^{-2\pi i/3}. \tag{13}$$

The appearance of cubic roots of the unity is the manifestation of the ternary symmetry of the problem. Now we introduce the generalized Bogoliubov transformation as

$$= T \tag{14}$$

To preserve the Boson commutation relations and to map $H_0(k)$ onto a diagonal matrix the column of the transformation matrix is written as $\begin{bmatrix} \lambda_i u_i \\ \mu_i u_i \end{bmatrix}$, where the coefficients λ_i and μ_i satisfy the hyperbolic orthonormalization conditions $|\lambda_i|^2 - |\mu_i|^2 = 1$, *etc.* So once three column vectors are found, the remaining three vectors are obtained by the action of $-\sigma_x$. In this way the transformation matrix T is obtained. So after the diagonalisation the Hamiltonian equation can be written as

$$H_k = \frac{9}{2} S^2(-J_1 - \sqrt{3}D_1) + 3hS + \frac{3S}{2}\sum_k \left[\psi_k^{\dagger} H_D \psi_k - 3C_1\right] \tag{15}$$

or

$$H_k = \frac{9}{2} S^2(-J_1 - \sqrt{3}D_1) + 3hS + 3S \sum_{k,L=1,2,3} \omega_L A_L^{\dagger} A_L + \frac{3S}{3}\sum_k (\omega_1 + \omega_2 + \omega_3 - 3C_1), \tag{16}$$

where

$$\omega_i = \sqrt{[C_1 + \rho_i(C_2 + C_3)][C_1 + \rho_i(C_2 - C_3)]}, \tag{17}$$

and

$$\rho_1 = z + z^*, \quad \rho_2 = zj + z^* j^2, \quad \rho_3 = z^* j + zj^2. \tag{18}$$

A three-dimensional excitation spectrum has been drawn in the Figure 2. It is seen that the excitation spectrum is real and positive over the Brillouin zone. There is the gap in the excitation spectra which has been calculated as

$$\omega_1^{(0,0)} = \sqrt{\frac{h}{3S}(-3J + \sqrt{3}D - \frac{h}{3S})},$$

$$\omega_{2,3}^{(0,0)} = \sqrt{\frac{1}{2}(\sqrt{3}D + \frac{h}{3S})(-3J + \sqrt{3}D - \frac{h}{3S})}, \tag{19}$$

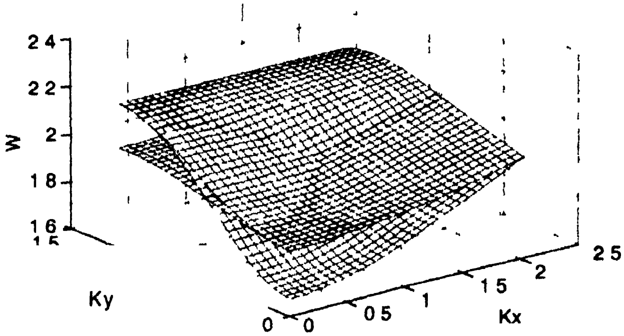

Figure 2. The three dimensional excitation spectra for $D = 0.3$ and $h = 1$ for $S = 0.5$.

The ground state energy including the zero point motion is

$$\frac{E_0}{J_1(\text{Bond})} = \frac{1}{2}S^2(-J_1-\sqrt{3}D_1)+\frac{hS}{2}+\frac{S}{2N}\sum(\omega_1+\omega_2+\omega_3)+\frac{S}{2}(-J_1-\sqrt{3}D_1+\frac{h}{3}) \,. \tag{20}$$

In the above expression, the last two terms give the quantum correction to the classical ground state energy. In the Figure 3(a) we plot the ground state energy as a function of D and it is observed that total ground state energy decreases as D increases.

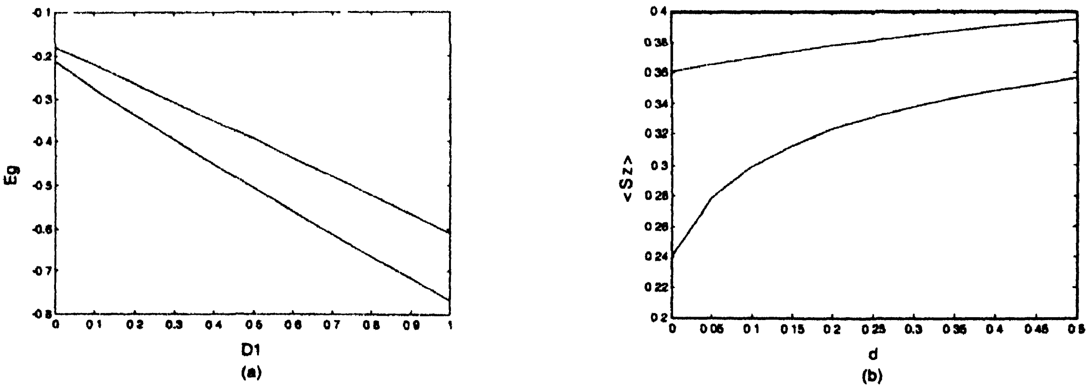

Figure 3. (a) Variation of ground state energy w.r.t. D at $h = 0$ (upper) and $h = -1.0$ (lower); (b) the variation of the sublattice magnetization with the DM interaction for $h = 0$ (lower curve) and for $h = -0.3$ (for upper curve). $S = 1/2$ value is considered.

There is also a reduction in the ground state sublattice magnetization due quantum mechanical fluctuations which is calculated per site as

$$2 \quad 2N \sum_{l,k} \quad \omega_l(k) \tag{21}$$

In the Figure 3(b) we plot the sublattice magnetization as a function of D and it is observed that this also increases as D increases.

4. Conclusion

In the previous section, we have studied the triangular lattice with spin wave theory. These lattices have been widely studied with Heisenberg Hamiltonian. But our calculation includes the anisotropic DM interaction. So the models become interesting because these are frustrated as well as anisotropic. The results are very much interesting because ground state energy and the reduction in sublattice magnetization reduces as the strength of DM interaction increases. So, the effect of this anisotropic interaction is to reduce the effect of quantum fluctuation in the triangular lattice. There are some magnetic systems, which are frustrated and no conclusion can be drawn about the ground state with the isotropic Heisenberg Hamiltonian. In these cases, due to large quantum fluctuation, the ground state is highly degenerate. But our calculation concludes that DM interaction reduces the quantum fluctuation and 120° ordering is favored.

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